数理解析研究所講究録
469巻 1982年 15-25

On the Dynamic and Ergodic Properties of the XY-Model.

Eytan Barouch

Research Institute for Mathematical Sciences
Kyoto University , Kyoto Japan and

Clarkson College of Technology
Potsdam, N.Y. 13676, U.S.A.

I. Introduction.

Recently,[1] the dynamic properties of the XY-model[2] received much attention within the role of the model as a non-trivial many-body dynamical spin system, whose time dependent properties can by studied exactly. It is well known[3] that the magnetization in the z direction is non-ergodic, and contains an explicit "memory" function. However, a single perturbation[4] does approach its equilibrium limit, which leads to the interpretation that the XY-chain acts like a "heat bath" on the local impurity.

A natural question rises in view of these results, namely how big can the "impurity" be while still approaching its equilibrium limit. It is the purpose of this note to address this question via an exlicit calculation. It is found that when the perturbation's size is comparable to the chain's size the system is not ergodic. When the perturbation is of a finite size, thermal equilibrium is always achieved. The situation is more complicated when the pertubation size is large but much smaller than the chain size.

II. Formulation

Define the XY-Hamitonian as

$$\mathcal{H}_o = -\frac{1}{2} \sum_{j=1}^{N-1} [(1+\gamma)\sigma_j^x \sigma_{j+1}^x + (1-\gamma)\sigma_j^y \sigma_{j+1}^y] \qquad (2.1)$$

with σ_j^x, σ_j^y, σ_j^z being the standard Pauli spin matrices. Also define the perturbation $\mathcal{H}_p$ as

$$\mathcal{H}_p = - \sum_{j=1}^{n} \sigma_j^z \qquad (2.2)$$

with $0 \leqslant n \leqslant N$, and the time dependent field as

$$h(t) = \begin{cases} h \geqslant 0 & t \leqslant 0 \\ 0 & t > 0 \end{cases} \qquad (2.3)$$

In other words, we assume that at $t \leqslant 0$ the system is at thermal equilibrium with a heat bath at temperature β^{-1}, and at $t = 0$ the external field is turned off. The initial density operator ρ is then defined by

$$\rho_N = Z^{-1} \exp\{-\beta[\mathcal{H}_o + h\mathcal{H}_p]\} \qquad (2.4)$$

with Z being the partition function defined by $\mathrm{tr}\rho_N = 1$, and the expected value $\langle Q \rangle$ of an operator Q is given by

$$\langle Q \rangle_N = \mathrm{tr}(\rho_N Q) \qquad (2.5)$$

The expected value of the perturbation at time t is the magnetization of this impurity at time t given per site as

$$\bar{m}_z(t) = \frac{1}{n} \sum_{j=1}^{n} \langle \rho_N \exp(i\mathcal{H}_o t)\sigma_j^z \exp(-i\mathcal{H}_o t) \rangle_N \qquad (2.6)$$

We first take the thermodynamic $(N \to \infty)$ limit, use the fact that the one-dimension XY chain does not have a long range order at any finite temperature and ask for which n does $\bar{m}_z(t)$ as defined by (2.6) approaches 0 as $t \to \infty$. Previous cases are $n = N$, $n = 1$, $n = 0$. In the following $\bar{m}_z(t)$ is computed explicitly for any n. Since it has been demonstrated that thermalization information is independent of γ as long as $\gamma \neq 1$, we specialize to the simpler case $\gamma = 0$ for mathematical convenience. Extension to $\gamma \neq 0$ is straightforward, somewhat more elaborate but contains no new information.

III. Computation of $\bar{m}_z(t)$.

The Hamiltonians $\mathcal{H}_o$, $\mathcal{H}_p$ (with $\gamma = 0$) can be written in terms of Fermion operators as

$$\mathcal{H}_o = -\sum_{j=1}^{N-1} \{C_j^+ C_{j+1} - C_j C_{j+1}^+\} \tag{3.1}$$

$$\mathcal{H}_p = -2\sum_{j=1}^{n} \{C_j^+ C_j - 1/2\} \tag{3.2}$$

and define $b = 2h$. Using the definitions (3.1), (3.2) and (2.6), we obtain

$$\bar{m}_z(t) = \frac{1}{n}\sum_{j=1}^{n} \langle \sigma_j^z(t) \rangle \quad . \tag{3.3}$$

and with

$$\langle C_j^+ C_j \rangle_t \equiv \frac{1}{2}\{1 + \langle \sigma_j^z(t) \rangle\} \tag{3.4}$$

we rewrite (3.3) as

$$\bar{m}_z(t) = \frac{2}{n} \sum_{j=1}^{n} \langle c_j^+ c_j \rangle_t - 1 \tag{3.5}$$

with $\langle c_j^+ c_j \rangle_t$ given explicitly by

$$\langle c_j^+ c_j \rangle_t = \mathrm{Tr}[c_j^+ c_j \exp[it\mathcal{H}_o] \exp[-\beta(\mathcal{H}_o + h\mathcal{H}_1)] \exp[-it\mathcal{H}_o]] \times \{\mathrm{Tr}[\exp(-\beta[\mathcal{H}_o + h\mathcal{H}_1])]\}^{-1} \tag{3.6}$$

The computation of the expected value at (3.6) is performed using the following steps :

(i) Transform $\mathcal{H}_o$ into a diagonal form

(ii) "Evolve" c_j^+ and c_j

(iii) Transform back, so $\mathcal{H}_o + h\mathcal{H}_1$ remains invariant

(iv) Diagonalize $\mathcal{H}_o + h\mathcal{H}_1$ and compute corresponding expected values.

We now proceed to perform these steps :

(i) Define new Fermion operators η_q by

$$c_m = N^{-1/2} e^{-i\pi/4} \sum_q e^{iqm} \eta_q \tag{3.7}$$

with

$$q = \frac{2s\pi}{N}, \quad s = 0, 1, 2, \ldots N-1 . \tag{3.8}$$

With this transformation $\mathcal{H}_o$ takes the form

$$\mathcal{H}_o = -2 \sum_q \cos q \, (\eta_q^+ \eta_q - 1/2) + O(N^{-1}) \tag{3.9}$$

(ii) The "evolved" operator $c_j^+ c_j$ at time t takes the form

$$(C_j^+C_j)_t = \exp[2it \sum_q \cos q\ \eta_q^+ \eta_q]\{\frac{1}{N} \sum_{q'q''} e^{ij(q'-q'')} \eta_{q''}^+ \eta_{q'}\}$$

$$*\exp[-2it \sum_{q_1} \cos q_1\ \eta_{q_1}^+ \eta_{q_1}] \qquad (3.10)$$

In other words the evolved operator $(C_j^+C_j)_t$ can be written as in terms of the operators η_q , η_q^+ and the explicit time t as

$$(C_j^+C_j)_t = \frac{1}{N} \sum_{p,p'} \exp\{i[2t(\cos p'-\cos p)+j(p-p')]\} \eta_{p'}^+ \eta_p \qquad (3.11)$$

(iii) Since the transformation (3.7) is cononical, we can easily express η_q in terms of the original Fermi operators C_j as

$$\eta_{p'}^+ \eta_p = \frac{1}{N} \sum_{m,m'=1}^{N} e^{i(p'm'-pm)} C_{m'}^+ C_m \qquad (3.12)$$

and the evolved operator $(C_j^+ C_j)_t$ is then given by

$$(C_j^+C_j)_t = \sum_{m,m'=1}^{N} \{[\frac{1}{N} \sum_p e^{i[-2t\cos p + p(j-m)]}]$$

$$\times[\frac{1}{N} \sum_{p'} e^{i[2t\cos p' + p'(m'-j)]}] C_{m'}^+ C_m\} \qquad (3.13)$$

Define the function $F(t,\ell)$ by

$$F(t,\ell) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i[2t\cos p + p\ell]}\, dp = i^\ell J_\ell(2t) \qquad (3.14)$$

with $J_\ell(2t)$ be Bessel's function of order ℓ , and it is elementary to verify that each term in the square brackets in (3.13) tends to $F(t,\ell)$ asymptotically as $N \to \infty$. Even though it is premature to take the thermodynamic limit at this stage, it can be taken for the above functions, at least for convenience, with the understanding that $J_\ell(2t)$ is at present a notation for the sum at (3.14) and not the integral.

We thus rewrite the evolved operator at time t as :

$$(C_j^+ C_j)_t = \sum_{m,m'} e^{i\frac{\pi}{2}(m'-m)} J_{m-j}(2t)\, J_{m'-j}(2t)\, C_{m'}^+ C_m \qquad (3.15)$$

with the expected value of $\bar{m}_z(t)$ given by

$$\bar{m}_z(t) = \frac{1}{n} \sum_{j=1}^{N} \sum_{m,m'=1}^{N} e^{i(\pi/2)(m'-m)} J_{m-j}(2t)\, J_{m'-j}(2t)\, E_{mm'} \qquad (3.16)$$

with the expected value $E_{m,m'}$ given by

$$E_{mm'} = \frac{\mathrm{tr}\{C_{m'}^+ C_m \;\; \mathrm{expt}[-\beta(\mathcal{H}_o + h\mathcal{H}_p)]\}}{\mathrm{tr}\{\exp[-\beta(\mathcal{H}_o + h\mathcal{H}_p)]\}} \qquad (3.17)$$

Thus, calculation of $E_{mm'}$ completes the explicit, exact computation of $\bar{m}_z(t)$. This is done in the forthcoming subsection (iv)

(iv) In Principle, the computations of $E_{m,m'}$ is straight forward, however the actual expressions do become rather cumbersome.

Since $\mathcal{H}_o$ and $\mathcal{H}_p$ are both quadratic structures in Fermion operators, we know that there exists a unitary transformation and new Fermion operators ψ_k, ψ_k^+ in which $\mathcal{H}$ is diagonal. More precisely we have the following relations

$$-\mathcal{H} \equiv -(\mathcal{H}_0 + b\mathcal{H}_p) = \sum_{j,k} C_j^+ B_{jk} C_k + \text{Const.} \tag{3.18}$$

with $B_{j,k} = 1$ if $j = k \pm 1$, $B_{jj} = b$ if $j \leq n$, and $B_{j,k} = 0$ otherwise.

$$C_m = \sum_k U_{mk} \psi_k \ , \quad C_{m'}^+ = \sum_\ell U_{m'\ell}^* \psi_\ell^+ \tag{3.19}$$

and the Hamiltonian is given by

$$-\mathcal{H} = \sum_k \Lambda_k \psi_k^+ \psi_k + \text{Const.} \tag{3.20}$$

with ψ_k, ψ_k^+ defined by (3.19) and Λ_k being the eigenvalues of the matrix B defined by (3.18). The expected value $E_{m,m'}$ thus takes the form

$$E_{m,m'} = \sum_{k,\ell} U_{m',\ell}^* U_{mk} \frac{\mathrm{tr}\{\psi_\ell^+\psi_k \exp[\beta \sum_{j=1}^{N} \Lambda_j \psi_j^+ \psi_j]\}}{\mathrm{tr}\{\exp[\beta \sum_j \Lambda_j \psi_j^+ \psi_j]\}}$$

$$= \sum_{k,} U_{m',k}^* U_{mk} (1 + e^{\beta\Lambda k})^{-1} \tag{3.21}$$

Equation (3.21) reduces to computation of $E_{m,m'}$ to the eigenvalues problem of the matrix B, whose eigenvector components are given by the coefficients U_{jk}.

Define the function $D_N(X)$ by

$$D_N(X) = \det (B - X I) \tag{3.22}$$

Clearly, the N zeros of $D_N(X)$ are the N eigenvalues Λ_j. Furthermore, due to the absence of translation invariance, the recursion relation for $D_N(X)$ are non-uniform, namely

$$D_k = (b - X)\, D_{k-1} - D_{k-2} \qquad 2 \le k \le n$$

$$D_\ell = - X\, D_{\ell-1} - D_{\ell-2} \qquad n+1 \le \ell \le N \tag{3.23}$$

and (3.23) can be solved exactly, with the explicit solution given by

$$D_N(X) = A(X)\, Z_+^{N-n}(X) + B(X)\, Z_-^{N-n}(X) \tag{3.24}$$

with

$$Z_\pm(X) = \frac{-X \pm [X^2 - 4]^{1/2}}{2} \tag{3.25}$$

$$A(X) = (X^2 - 4)^{-1/2} \left\{ \left[\frac{-X + (X^2-4)^{1/2}}{2} \right] P_n(X) - P_{n-1}(X) \right\} \tag{3.26}$$

$$B(X) = (X^2 - 4)^{-1/2} \left\{ \left[\frac{X + (X^2-4)^{1/2}}{2} \right] P_n(X) + P_{n-1}(X) \right\} \tag{3.27}$$

$$P_m(X) = [(X - b)^2 - 4]^{-1/2} \left\{ \left[\frac{-(X-b)+[(X-b)^2 - 4]^{1/2}}{2} \right]^{n+1} - \left[\frac{-(X-b)-[(X-b)^2 - 4]^{1/2}}{2} \right]^{n+1} \right\} \tag{3.28}$$

The coefficients $U_{jm} \equiv U_j(\Lambda_m)$ are determined in a similar manner from the equation

$$U_{j-1}(\Lambda_m) + t_j\, U_j(\Lambda_m) + U_{j+1}(\Lambda_m) = \Lambda_m U_j(\Lambda_m) \tag{3.29}$$

with

$$\sum_{j=1}^{N} | U_j(\Lambda_m)|^2 = 1 \tag{3.30}$$

and t_j is given by

$$t_j = \begin{cases} b & j \le n \\ 0 & j > n \end{cases} \tag{3.31}$$

Define the functions $\Theta_\pm(\Lambda_m)$, $\Phi_\pm(\Lambda_m)$

$$\Theta_\pm(\Lambda_m) = \frac{-(b-\Lambda_m) \pm [(b-\Lambda_m)^2 - 4]^{1/2}}{2} \tag{3.32}$$

$$\Phi_\pm(\Lambda_m) = \Theta_\pm(\Lambda_m, b=0) \tag{3.33}$$

In terms of (3.32) and (3.33), the coefficients $U_j(\Lambda_m)$ are given by

$$U_j(\Lambda_m) \begin{cases} A(\Lambda_m)\,[\Theta_+^j(\Lambda_m) - \Theta_-^j(\Lambda_m)] & i \le j \le n \\ A(\Lambda_m)[C(\Lambda_m)\,\Phi_+^{j-1}(\Lambda_m) + D(\Lambda_m)\,\Phi_-^{j-n}(\Lambda_m)] & n \le j \le N \end{cases} \tag{3.34}$$

where $A(\Lambda_m)$ is determind by the normalization condition, and $C(\Lambda_m)$ and $D(\Lambda_m)$ are given explicity by

$$C(\Lambda_m) = (\Lambda_m^2 - 4)^{-1/2}[\Theta_+^n(\Theta_+-\Phi_-) - \Theta_-^n(\Theta_- - \Phi_-)]$$

$$D(\Lambda_m) = (\Lambda_m^2 - 4)^{-1/2}[\Theta_+^n(\Phi_+-\Theta_+) - \Theta_-^n(\Phi_+ - \Theta_-)] \tag{3.35}$$

Note that at $n = j$ the two expressions of $U_n(\Lambda_m)$ at (3.34) are identical. Also note that $U_j(\Lambda_m)$ is proportional to $A(\Lambda_m)$ for all $j = 1, 2, \cdots N$.

Thus $|A(\Lambda_m)|^2$ given explicity by the relation

$$|A(\Lambda_m)|^2 = \Big\{\sum_{j=1}^{n}|\Theta_+^j(\Lambda_m) - \Theta_-^j(\Lambda_m)|^2 + \sum_{j=n+1}^{N}|C(\Lambda_m)\,\Phi_+^{j-n}(\Lambda_m) + D(\Lambda_m)\Phi_-^{j-n}(\Lambda_m)|^2\Big\}^{-1} \tag{3.36}$$

We can now express $E_{m,m'}$ of (3.21) as a contour integral where the contour surrounds the zeros of $D_N(X)$ given by (3.24) but avoiding the zeros of $1 + \exp(\beta X)$. In other words $E_{m\,m'}$ is given by

$$E_{mm'} = \frac{1}{2\pi i} \oint \frac{D_N'(X)\ U^*_{m'}(X)\ U_m(X)}{D_N(X)[1+\exp(\beta X)]}\ dX \tag{3.37}$$

with $D_N(X)$ given by (3.24), $U_m(X)$ given by (3.34). Substitution of (3.37) in (3.16) yields the desired answer. Explicitly, $\bar{m}_z(t)$ is given by

$$\bar{m}_z(t) = \frac{1}{n} \sum_{j=1}^{n} \frac{1}{2\pi i} \oint \frac{d\zeta}{1+e^{\beta\zeta}} \left| G_j(\zeta,t) \right|^2 \frac{D'_N(\zeta)}{D_N(\zeta)} \tag{3.38}$$

and $G_j(\zeta,t)$ is given by

$$G_j(\zeta,t) = \frac{1}{N} \sum_p e^{-i(2t\cos p - pj)} V_N(p,\zeta) \tag{3.39}$$

$$V_N(p,\zeta) = \sum_{m=1}^{N} e^{-ipm} U_m(\zeta) \tag{3.40}$$

with $U_j(\zeta)$ given by (3.34) and $D_N(\zeta)$ by (3.24). Note that the thermodynamic limit of (3.38)-(3.40) can be taken directly, from which the following conclusions can be drawn (Yes or No represents thermalization or non thermalization) :

(i) $N \to \infty$, $t \to \infty$, n finite Yes

(ii) $N \to \infty$, $n = O(N)$, $t \to \infty$: NO

(iii) $N \to \infty$, $t \to \infty$, $n \to \infty$: Yes

(iv) $N \to \infty$, $(n,t) \to \infty$: Needs further analysis.

References

[1] M. Dresden, Physica 110 A (1982), 1-40.

[2] E. Lieb, T. Schultz and D. Mattis, Annals of Phys. 16 (1961), 407-466.

[3] E. Barouch, B.M. McCoy and M. Dresden, Phys. Rev. A2 (1970), 1075-1092.

[4] D.E. Abraham, E. Barouch, G. Gallavotti and A. Martin-Löf, Studies in Appplied Math. 50 (1971), 121-131 ; 51 (1972), 211-218.